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Crystallographic report

Crystal structure of a two-dimensional coordination polymer: dizinc diterephthalate pyrazine dihydrate

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A two-dimensional coordination polymer $[Zn_2(tp)_2(pz)(H_2O)_2]_n$ (tp = terephthalate, pz = pyrazine) has been synthesized by the hydrothermal reaction of zinc terephthalate and pyrazine. The Zinc(II) centre is in a distorted pyramidal geometry, being coordinated by one water molecule, one nitrogen atom from a bridging pz and two different bridging tp ligands, one chelating and the other monodentate. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: zinc; terephthalate; pyrazine; crystal structure; coordination polymer

COMMENT

Rigid ligands, such as benzene polycarboxylic acids and heterocyclic aromatic compounds, are known as good candidates for assembling coordination polymers.[1–5] The coordination polymers formed by d^{10} metal, such as Zinc(II), and rigid aromatic carboxylate groups often exhibit intriguing photoluminescent properties.[1–4] Here, we report the synthesis and crystal structure of a two-dimensional (2D) coordination polymer, $[Zn_2(tp)_2(pz)(H_2O)_2]_n$ (**1**; tp = terephthalate, pz = pyrazine). Crystallography shows the Zinc(II) centre to exist in a distorted trigonal pyramidal environment defined by one oxygen atom from a coordinated water, one nitrogen atom of a bridging pyrazine and three oxygen atoms belonging to two different bridging carboxylate groups, as shown in Fig. 1. The resulting assembly is a 2D layer structure.

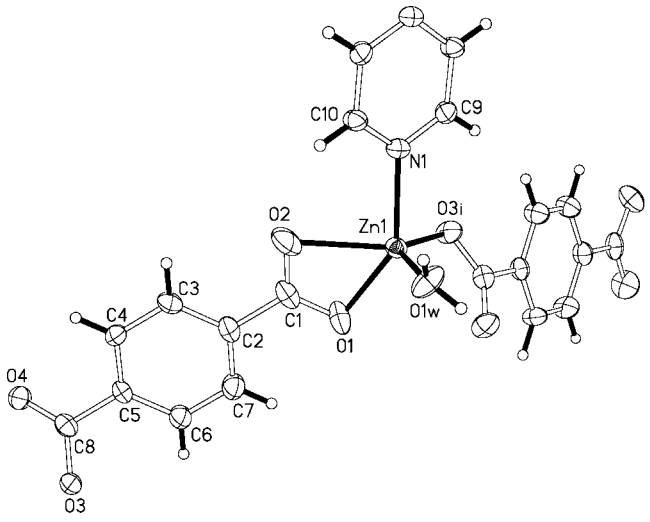

Figure 1. ORTEP plot showing the coordination environment of zinc atom at the 50% probability level. Key geometry parameters: Zn1–O1w 1.956(3), Zn1–O1 2.051(3), Zn1–O2 2.317(4), Zn1–N1 2.119(4), Zn1–$O3^i$ 1.964(3) Å; O1w–Zn1-$O3^i$ 124.21(16), O1w–Zn1–O1 103.21(16), $O3^i$–Zn1–O1 102.18(14), O1w–Zn1–N1 96.84(16), $O3^i$–Zn1–N1 90.80(14), O1–Zn1–N1 143.60(15), O1w–Zn1–O2 103.57(16), $O3^i$–Zn1–O2 132.10(14), O1–Zn1–O2 59.77(14), N1–Zn1–O2 86.26(14)°. Symmetry operation: i, $-x+2$, $y+1/2$, $-z+1/2$.

EXPERIMENTAL

Powders of zinc terephthalate DMF solvate[6] and pyrazine in 1:1 molar ratio in water (15 ml) were transferred and sealed in a 30 ml

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Teflon-lined stainless steel container. The container was heated to 180 °C and held at that temperature for 1 day, then cooled to 100 °C at a rate of 5 °C h^{-1}, held for 10 h, followed by further cooling to 30 °C at a rate of 5 °C h^{-1}. Colourless crystals of **1** were collected. Intensity data were collected at 298 K on a Bruker Smart Apex CCD diffractometer for a crystal $0.10 \times 0.14 \times 0.42$ mm^3 $C_{10}H_8NO_5Zn$, $M = 287.54$, monoclinic, $P2_1/c$, $a = 5.2849(4)$, $b = 18.4302(12)$, $c = 10.7757(7)$ Å, $\beta = 94.012(1)^o$, $V = 1047.00(12)$ $Å^3$, $Z = 4$; 2380 unique data ($\theta = 28.2^o$), 2136 data with $I > 2\sigma(I)$. $R_1 = 0.063$, $wR_2 = 0.139$; $\rho_{max} = 1.06$ e $Å^{-3}$. Programs used: SHELXL and ORTEP. CCDC deposition number: 208 984.

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